



STIC Search Report

EIC 1700

STIC Database Tracking Number: 99735

TO: Ling Xu
Location: CP3 11D28
Art Unit: 1775
July 29, 2003

Case Serial Number: 09/614511

From: John Calve
Location: EIC 1700
CP3/4-3D62
Phone: 703-308-4139

John.calve@uspto.gov

Search Notes

Ling,

I didn't find any records with substitutions on the 3rd, 4th and 5th positions. The best record I found has a methyl group on the 3rd position and a halogen on the 5th position. I printed out a few records of the art that is closest to applicants.

John

99735

SEARCH REQUEST FORM

Scientific and Technical Information Center

Examiner# : 77924

Art Unit : 1775

Phone Number: 305-0395

Date: 7/28/2003

Serial Number: 09/614,511

MailBox & Bldg/Room Location: CP3 11d28

Results Format Preferred (circle): Paper Disk E-mail

If more than one search is submitted, please prioritize searches in order of need.

Please provide a detailed statement of the search topic, and describe as specifically as possible the subject matter to be searched. Include the elected species or structures, keywords, synonyms, acronyms, and registry numbers, and combine with the concept or utility of the invention. Define any terms that may have a special meaning. Give examples or relevant citations, authors, etc., if known. Please attach a copy of the coversheet, pertinent claims, and abstract.

Title of Invention:

Material for use in a light-emitting device and highly efficient electroluminescent device

Inventors (please provide full names):

Wanda andreoni, Alessandro Curioni

Earliest Priority Filing Date: 7/12/1999 ← EPO 99113398

For Sequence Searches Only Please include all pertinent information (parent, child, divisional, or issued patent numbers) along with the appropriate serial number.

Please search the organic material having the Alq3 as a base unit and is substituted solely in the 3, 4 and 5 positions as described in claim 8, please search the material with electroluminescent device, EL device, light emitting device. Specific substituents are listed in claims 9-14.

Please call me if you have any questions.

Thanks

Wing Ku 1-9



STIC Search Results Feedback Form

EIC17000

Questions about the scope or the results of the search? Contact *the EIC searcher or contact:*

Kathleen Fuller, EIC 1700 Team Leader
308-4290, CP3/4-3D62

Voluntary Results Feedback Form

➤ I am an examiner in Workgroup: Example: 1713

➤ Relevant prior art **found**, search results used as follows:

- ☐ 102 rejection
- ☐ 103 rejection
- ☐ Cited as being of interest.
- ☐ Helped examiner better understand the invention.
- ☐ Helped examiner better understand the state of the art in their technology.

Types of relevant prior art found:

- ☐ Foreign Patent(s)
- ☐ Non-Patent Literature
(journal articles, conference proceedings, new product announcements etc.)

➤ Relevant prior art **not found**:

- ☐ Results verified the lack of relevant prior art (helped determine patentability).
- ☐ Results were not useful in determining patentability or understanding the invention.

Comments:

Drop off or send completed forms to STIC/EIC1700 CP3/4 3D62



=> file reg

FILE 'REGISTRY' ENTERED AT 09:36:46 ON 29 JUL 2003
USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.
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Property values tagged with IC are from the ZIC/VINITI data file
provided by InfoChem.

STRUCTURE FILE UPDATES: 27 JUL 2003 HIGHEST RN 556005-78-8
DICTIONARY FILE UPDATES: 27 JUL 2003 HIGHEST RN 556005-78-8

TSCA INFORMATION NOW CURRENT THROUGH JANUARY 6, 2003

Please note that search-term pricing does apply when
conducting SmartSELECT searches.

Crossover limits have been increased. See HELP CROSSOVER for details.

Experimental and calculated property data are now available. See HELP
PROPERTIES for more information. See STNote 27, Searching Properties
in the CAS Registry File, for complete details:
<http://www.cas.org/ONLINE/STN/STNOTES/stnotes27.pdf>

=> d his

(FILE 'HOME' ENTERED AT 08:34:41 ON 29 JUL 2003)

FILE 'HCA' ENTERED AT 08:35:13 ON 29 JUL 2003

L1 119 S CURIONI ?/AU
L2 510 S ANDREONI ?/AU
L3 6 S L1 AND L2 AND ALQ3
SEL L3 1-6 RN

FILE 'REGISTRY' ENTERED AT 08:35:58 ON 29 JUL 2003

L4 6 S E1-E6
L5 3 S L4 AND 5-100/C

FILE 'LREGISTRY' ENTERED AT 08:36:48 ON 29 JUL 2003

L6 STR 136781-07-2
L7 STR L6

FILE 'REGISTRY' ENTERED AT 08:41:06 ON 29 JUL 2003

L8 1 S L7
L9 1874 S 12628?/RID
L10 260 S L9 AND 1-5/AL

FILE 'LREGISTRY' ENTERED AT 08:43:14 ON 29 JUL 2003

L11 STR L7

FILE 'REGISTRY' ENTERED AT 08:45:07 ON 29 JUL 2003

L12 19 S L11

FILE 'LREGISTRY' ENTERED AT 08:45:42 ON 29 JUL 2003

L13 STR L11

FILE 'REGISTRY' ENTERED AT 09:13:37 ON 29 JUL 2003

L14 19 S L11
L15 313 S L11 FULL
SAVE L15 LINGXU511/A

L16 3 S L13 SSS SAM SUB=L15
L17 65 S L13 SSS FULL SUB=L15
SAVE L17 LINGXU511A/A

FILE 'HCA' ENTERED AT 09:16:52 ON 29 JUL 2003
L18 89 S L17

FILE 'CAOLD' ENTERED AT 09:17:00 ON 29 JUL 2003
L19 1 S L17

FILE 'HCA' ENTERED AT 09:17:18 ON 29 JUL 2003

FILE 'REGISTRY' ENTERED AT 09:18:48 ON 29 JUL 2003
E 146162-48-3
L20 1 S L17 AND 146162-48-3
E 14752-00-2/RN
L21 1 S L17 AND 14752-00-2/RN
L22 63 S L17 NOT (L20 OR L21)

FILE 'HCA' ENTERED AT 09:20:41 ON 29 JUL 2003
L23 19 S L22

FILE 'LREGISTRY' ENTERED AT 09:21:43 ON 29 JUL 2003
E 292631-39-1/RN

FILE 'REGISTRY' ENTERED AT 09:25:09 ON 29 JUL 2003
E 292631-39-1/RN
L24 1 S E3

FILE 'LREGISTRY' ENTERED AT 09:28:02 ON 29 JUL 2003
L25 STR L13

FILE 'REGISTRY' ENTERED AT 09:32:41 ON 29 JUL 2003
L26 0 S L25 SSS SAM SUB=L15
L27 21 S L25 SSS FULL SUB=L15

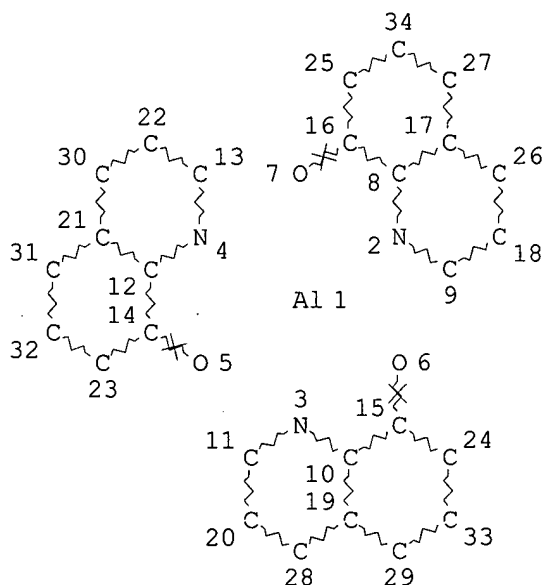
FILE 'HCA' ENTERED AT 09:33:56 ON 29 JUL 2003
L28 39 S L27

FILE 'REGISTRY' ENTERED AT 09:34:17 ON 29 JUL 2003
L29 20 S L27 NOT (L20 OR L21)

FILE 'HCA' ENTERED AT 09:34:40 ON 29 JUL 2003
L30 13 S L29
L31 9 S L30 AND 1907-2000/PY

FILE 'REGISTRY' ENTERED AT 09:36:46 ON 29 JUL 2003

=> d que stat L27
L11 STR



NODE ATTRIBUTES:

NSPEC	IS	RC	AT	1
NSPEC	IS	RC	AT	5
NSPEC	IS	RC	AT	6
NSPEC	IS	RC	AT	7

DEFAULT MLEVEL IS ATOM

DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:

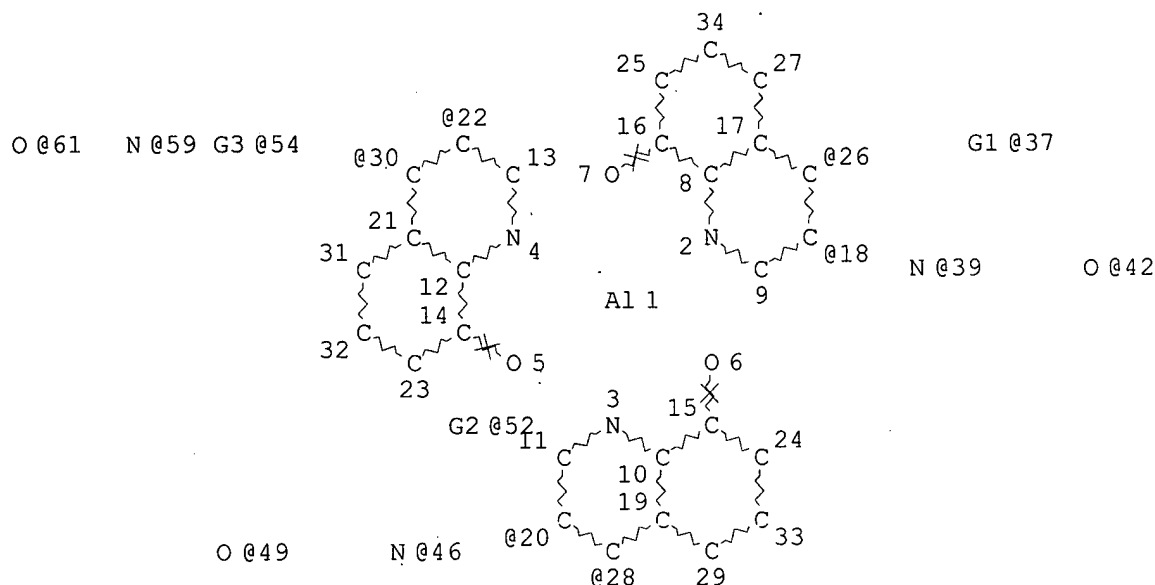
RING(S) ARE ISOLATED OR EMBEDDED

NUMBER OF NODES IS 34

STEREO ATTRIBUTES: NONE

L15 313 SEA FILE=REGISTRY SSS FUL L11

L25 STR



VAR G1=AK/39/42

VAR G2=AK/49/46

VAR G3=AK/59/61

VPA 37-18/26 U

VPA 52-20/28 U

VPA 54-22/30 U

NODE ATTRIBUTES:

NSPEC IS RC AT 1

NSPEC IS RC AT 5

NSPEC IS RC AT 6

NSPEC IS RC AT 7

CONNECT IS E2 RC AT 9

CONNECT IS E2 RC AT 11

CONNECT IS E2 RC AT 13

CONNECT IS E2 RC AT 32

CONNECT IS E2 RC AT 33

CONNECT IS E2 RC AT 34

DEFAULT MLEVEL IS ATOM

DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:

RING(S) ARE ISOLATED OR EMBEDDED

NUMBER OF NODES IS 43

STEREO ATTRIBUTES: NONE

L27 21 SEA FILE=REGISTRY SUB=L15 SSS FUL L25

100.0% PROCESSED 290 ITERATIONS

21 ANSWERS

SEARCH TIME: 00.00.01

=> file hca

FILE 'HCA' ENTERED AT 09:37:35 ON 29 JUL 2003

USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.

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FILE COVERS 1907 - 24 Jul 2003 VOL 139 ISS 5

FILE LAST UPDATED: 24 Jul 2003 (20030724/ED)

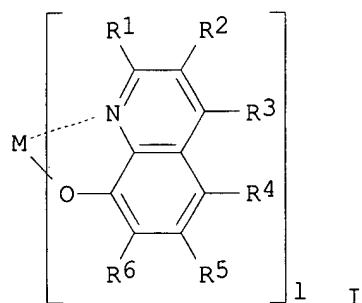
This file contains CAS Registry Numbers for easy and accurate substance identification.

=> d L31 1-9 cbib abs hitstr

L31 ANSWER 1 OF 9 HCA COPYRIGHT 2003 ACS on STN

133:244884 Organic electroluminescent component. Tsuge, Hodaka; Ishii, Satoshi; Shimada, Yoichi (Honda Motor Co., Ltd., Japan). Jpn. Kokai Tokkyo Koho JP 2000252072 A2 **20000914**, 28 pp. (Japanese).
CODEN: JKXXAF. APPLICATION: JP 1999-55905 19990303.

GI



AB The invention refers to an org. electroluminescent component comprising I [R1-6 = H, hydrocarbon or oxy group, where at least one is not H; M = metal; 1 = valence of M] in the luminescent layer.

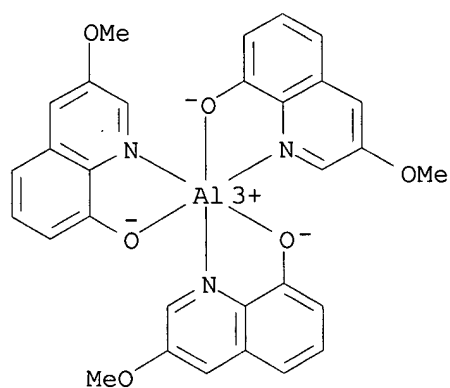
IT 292631-19-7 292631-20-0 292631-44-8
292631-45-9 292631-47-1 292631-48-2
292631-50-6 292631-64-2 292631-66-4
292631-68-6 292631-71-1 292631-85-7

RL: DEV (Device component use); MOA (Modifier or additive use); USES (Uses)

(org. electroluminescent component)

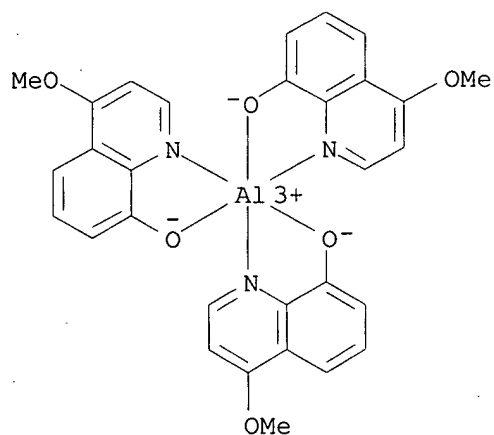
RN 292631-19-7 HCA

CN Aluminum, tris(3-methoxy-8-quinolinolato-.kappa.N1,.kappa.O8)- (9CI) (CA INDEX NAME)



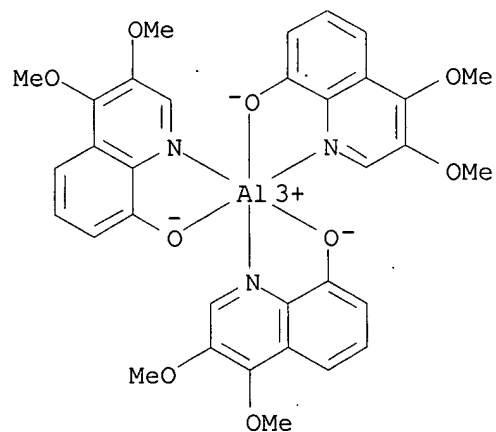
RN 292631-20-0 HCA

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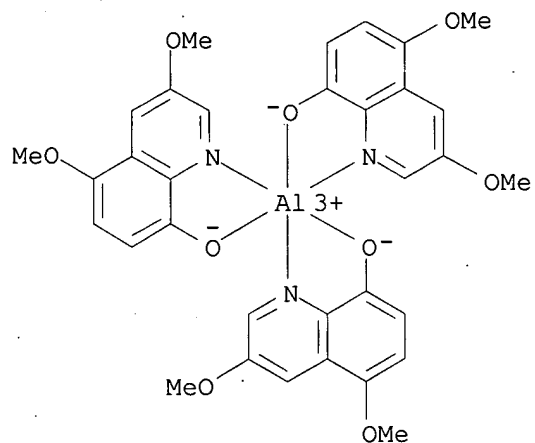
CN Aluminum, tris(3,4-dimethoxy-8-quinolinolato-.kappa.N1,.kappa.O8)- (9CI) (CA INDEX NAME)



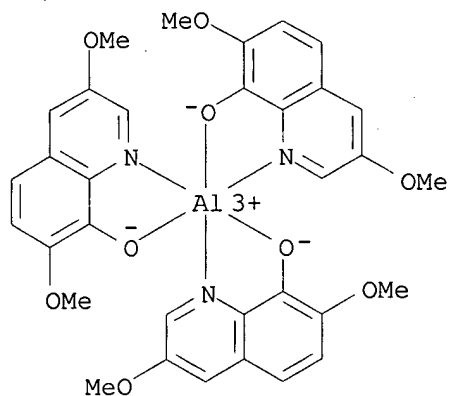
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CN Aluminum, tris(3,5-dimethoxy-8-quinolinolato-.kappa.N1,.kappa.O8)- (9CI)

(CA INDEX NAME)

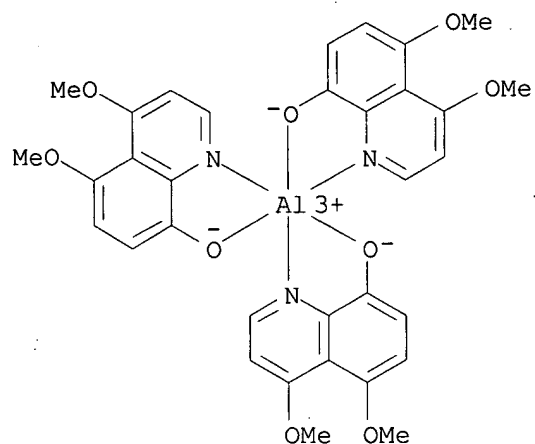


RN 292631-47-1 HCA

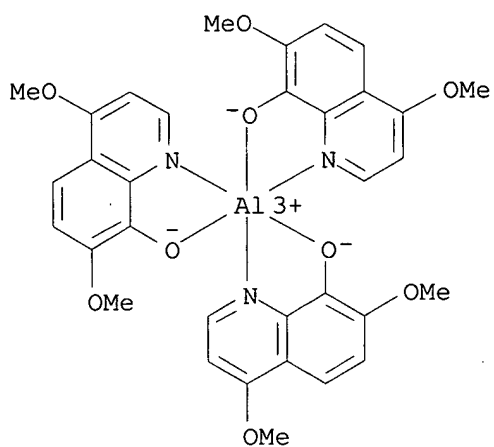
CN Aluminum, tris(3,7-dimethoxy-8-quinolinolato-.kappa.N1,.kappa.O8)- (9CI)
(CA INDEX NAME)

RN 292631-48-2 HCA

CN Aluminum, tris(4,5-dimethoxy-8-quinolinolato-.kappa.N1,.kappa.O8)- (9CI)
(CA INDEX NAME)

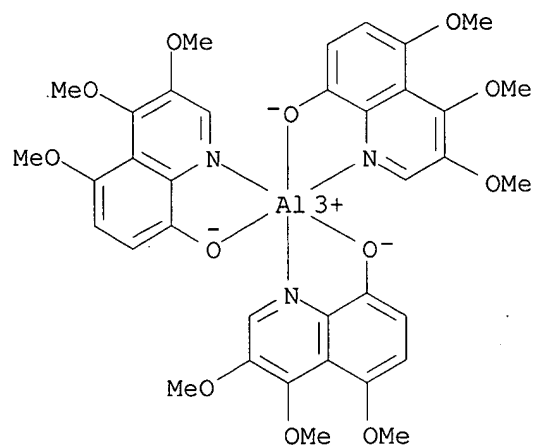


RN 292631-50-6 HCA

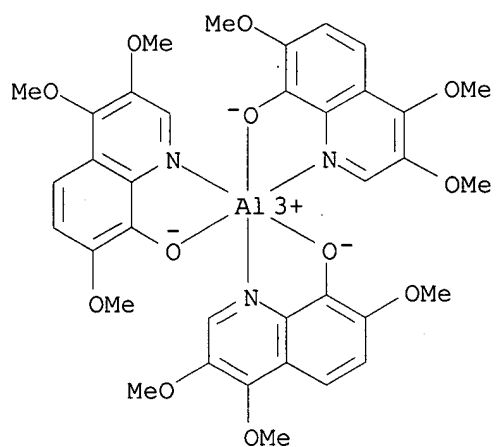
CN Aluminum, tris(4,7-dimethoxy-8-quinolinolato-.kappa.N1,.kappa.O8)- (9CI)
(CA INDEX NAME)

RN 292631-64-2 HCA

CN Aluminum, tris(3,4,5-trimethoxy-8-quinolinolato-.kappa.N1,.kappa.O8)-
(9CI) (CA INDEX NAME)

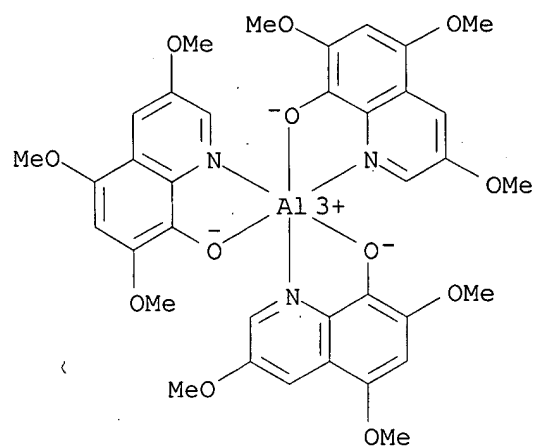


RN 292631-66-4 HCA

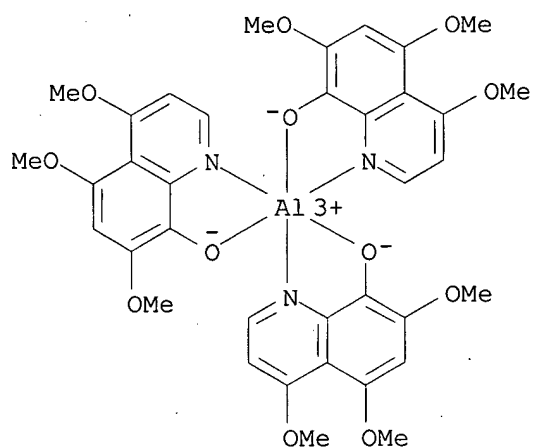
CN Aluminum, tris(3,4,7-trimethoxy-8-quinolinolato-.kappa.N1,.kappa.O8)-
(9CI) (CA INDEX NAME)

RN 292631-68-6 HCA

CN Aluminum, tris(3,5,7-trimethoxy-8-quinolinolato-.kappa.N1,.kappa.O8)-
(9CI) (CA INDEX NAME)

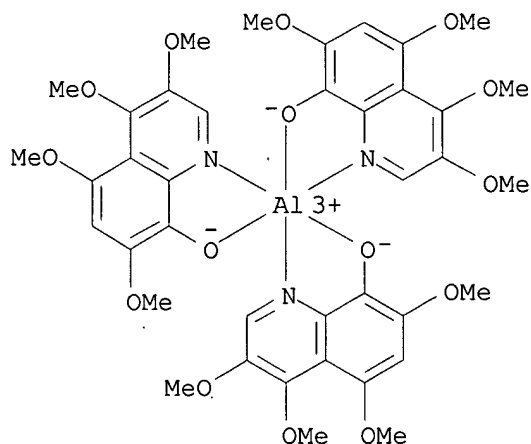


RN 292631-71-1 HCA

CN Aluminum, tris(4,5,7-trimethoxy-8-quinolinolato-.kappa.N1,.kappa.O8)-
(9CI) (CA INDEX NAME)

RN 292631-85-7 HCA

CN Aluminum, tris(3,4,5,7-tetramethoxy-8-quinolinolato-.kappa.N1,.kappa.O8)-
(9CI) (CA INDEX NAME)



L31 ANSWER 2 OF 9 HCA COPYRIGHT 2003 ACS on STN

133:142404 Materials for organic electroluminescence: aluminum vs. boron.

Anderson, S.; Weaver, M. S.; Hudson, A. J. (Sharp Laboratories of Europe, Oxford, OX4 4GB, UK). Synthetic Metals, 111-112, 459-463 (English)

2000. CODEN: SYMEDZ. ISSN: 0379-6779. Publisher: Elsevier Science S.A..

AB The authors report the synthesis of B complexes 1-7 and their absorption and emission (photoluminescence and electroluminescence) characteristics in soln. and in the solid state. The authors compare their electronic properties to those of the Alq3 analogs, and use MO calcns. to rationalize the λ_{max} shifts caused by systematically substituting Me groups around the periphery of the 8-hydroxyquinoline ligand moiety.

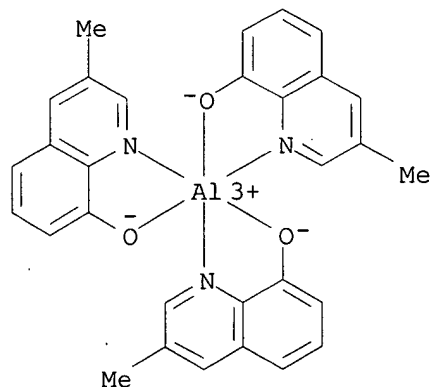
IT **136711-26-7P 136779-65-2P**

RL: DEV (Device component use); PRP (Properties); SPN (Synthetic preparation); PREP (Preparation); USES (Uses)

(materials for org. electroluminescence: aluminum vs. boron)

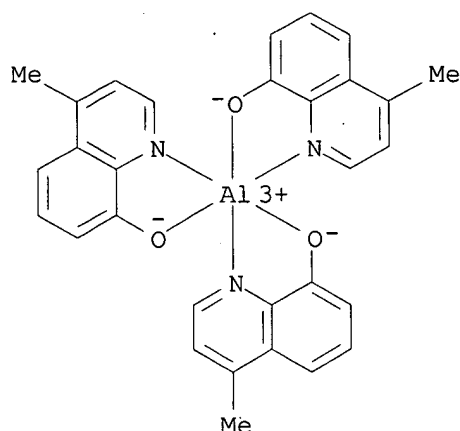
RN 136711-26-7 HCA

CN Aluminum, tris(3-methyl-8-quinolinolato-.kappa.N1,.kappa.O8)-, (OC-6-21)-(9CI) (CA INDEX NAME)



RN 136779-65-2 HCA

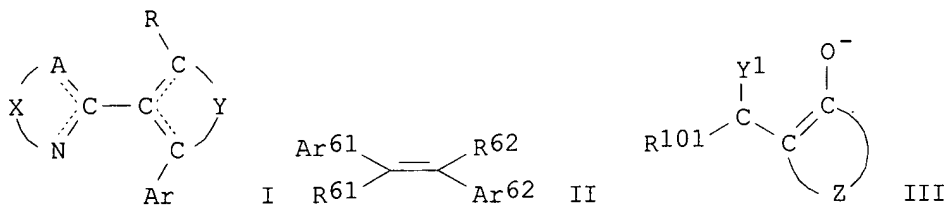
CN Aluminum, tris(4-methyl-8-quinolinolato-.kappa.N1,.kappa.O8)-, (OC-6-21)-(9CI) (CA INDEX NAME)



L31 ANSWER 3 OF 9 HCA COPYRIGHT 2003 ACS on STN

133:81409 Electroluminescent material, electroluminescent element and color conversion filter. Kita, Hiroshi; Suzuri, Yoshiyuki; Yamada, Taketoshi; Nakamura, Kazuaki; Ueda, Noriko; Okubo, Yasushi (Konica Corporation, Japan). Eur. Pat. Appl. EP 1013740 A2 **20000628**, 80 pp.
 DESIGNATED STATES: R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO. (English). CODEN: EPXXDW.
 APPLICATION: EP 1999-125813 19991223. PRIORITY: JP 1998-370452 19981225; JP 1999-246404 19990831.

GI



AB Electroluminescent materials are described which are based on derivs. of arom. heterocycles, binaphthyls, and triarylamines which include substituents (esp. biaryl substituents) contg. bonds capable of giving internal rotational isomerism, or on compds. described by the general formulas I (Ar = aryl; A = C, N, S or O; X = group of atoms necessary to form 5- or 6-member N contg. arom. heterocyclic ring; Y = group of atoms necessary to form 5- or 6-member arom. hydrocarbon or arom. heterocyclic ring, provided that the bond of C-N, C-A or C-C in the formula is a single or double bond; and R = H, substituent, or Ar) or II (Ar61 and Ar62 = each aryl or arom. heterocyclic; R61 and R62 = each H or substituent, provided that .gtoreq.1 of Ar61, Ar62, R61, and R62 = biaryl group contg. a bond capable of giving internal rotational isomerism or a group contg. such a biaryl group); rare earth metal complex fluorescent substances contg. at least an anionic ligand represented by the formula III (R101 = H or substituent; Y1 = O, S or N(R102); R102 = H or substituent; and Z = atoms forming a 4- to 8-membered ring) are also described. Electroluminescent elements comprising an electroluminescent material and a fluorescent substance emitting light having an emission max. at the wavelength different from that of light emitted from the electroluminescent material upon absorption of the light emitted from the electroluminescent material

are also described, as are color conversion filters comprising a fluorescent substance emitting light having an emission max. at 400-700 nm upon absorption of the light emitted from the electroluminescent material.

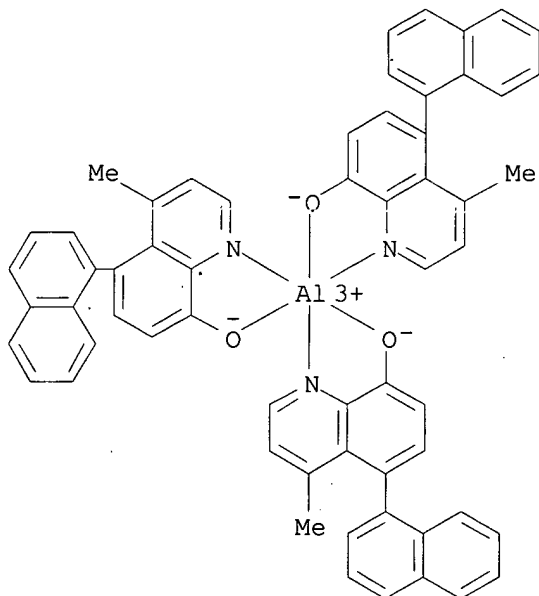
IT **278794-70-0**

RL: DEV (Device component use); USES (Uses)

(electroluminescent materials based on compds. including substituents with internal rotation isomers and rare earth complex-based fluorescent materials and electroluminescent elements and color conversion filters)

RN 278794-70-0 HCA

CN Aluminum, tris[4-methyl-5-(1-naphthalenyl)-8-quinolinolato-.kappa.N1,.kappa.O8]- (9CI) (CA INDEX NAME)



L31 ANSWER 4 OF 9 HCA COPYRIGHT 2003 ACS on STN

132:327205 A Matrix-Isolation Spectroscopic and Theoretical Investigation of Tris(8-hydroxyquinolinato)aluminum(III) and Tris(4-methyl-8-hydroxyquinolinato)aluminum(III). Kushto, Gary P.; Iizumi, Yasuhiro; Kido, Junji; Kafafi, Zakya H. (United States Naval Research Laboratory, Washington, DC, 20375, USA). Journal of Physical Chemistry A, 104(16), 3670-3680 (English) 2000. CODEN: JPCAFH. ISSN: 1089-5639. Publisher: American Chemical Society.

AB IR and luminescence of matrix-isolated and thin-film samples (both at 11 K) of tris(8-hydroxyquinolinato)aluminum(III) (Alq3) and tris(4-Me-8-hydroxyquinolinato)aluminum(III) (Almq3) were collected and compared to vibrational spectra generated by B3LYP based d. functional calcns. The present IR spectral results suggest that both Alq3 and Almq3 exist primarily in the meridional or C1 isomeric form with little or no spectral evidence for the presence of the alternate, facial (C3 symmetry) geometric isomer. Luminescence of these mols. isolated in an Ar matrix show vibronic structure in the emission band assocd. with the S1 .fwdarw. S0 transition.

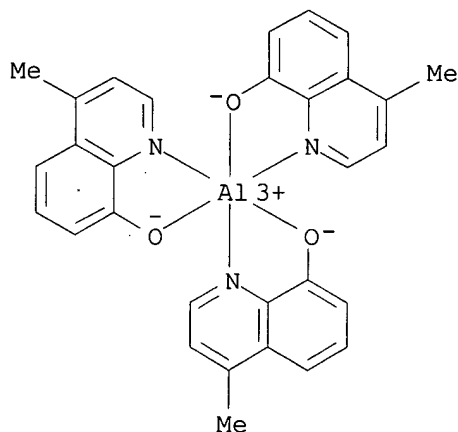
IT **136779-65-2**

RL: PEP (Physical, engineering or chemical process); PRP (Properties); PROC (Process)

(matrix-isolation IR and luminescence spectra and d. functional calcn. of aluminum hydroxyquinolinato and methylhydroxyquinolinato complexes)

RN 136779-65-2 HCA

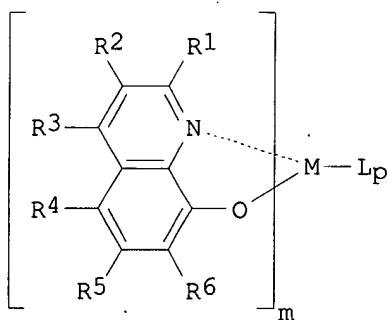
CN Aluminum, tris(4-methyl-8-quinolinolato-.kappa.N1,.kappa.O8)-, (OC-6-21)-
(9CI) (CA INDEX NAME)



L31 ANSWER 5 OF 9 HCA COPYRIGHT 2003 ACS on STN

131:250257 Organic electroluminescent device containing halogenated chelate complex. Terazono, Shinji; Asari, Goro; Takahashi, Akira (Asahi Glass Co., Ltd., Japan). Jpn. Kokai Tokkyo Koho JP 11260558 A2 **19990924** Heisei, 7 pp. (Japanese). CODEN: JKXXAF. APPLICATION: JP 1998-57132 19980309.

GI



AB The device contains an anode, a light-emitting layer, an interface org. layer, and a cathode, in which the interface layer contains a chelate complex I (R1-6 = H, halogen, alkyl, alkoxy, aryl, aryloxy, acyl, aralkyl; M = metal; m = 1-3 integer; L = alkoxy, aryloxy; p = 0, 1, 2; at least one of R1-6 = halogen). The device shows low emission voltage and high luminance with efficiency.

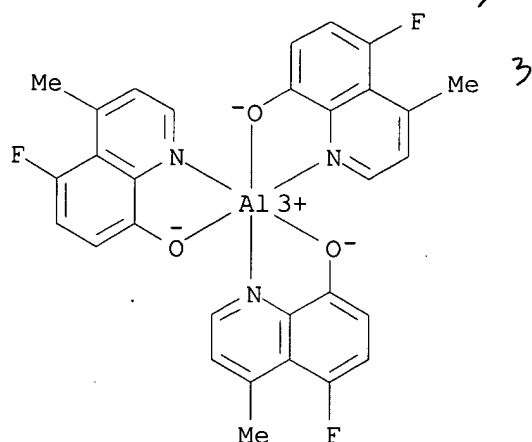
IT **244201-79-4**

RL: DEV (Device component use); MOA (Modifier or additive use); USES (Uses)

(org. electroluminescent device contg. halogenated chelate complex)

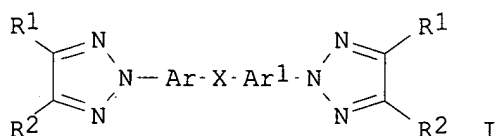
RN 244201-79-4 HCA

CN Aluminum, tris(5-fluoro-4-methyl-8-quinolinolato-.kappa.N1,.kappa.O8)-
(9CI) (CA INDEX NAME)



L31 ANSWER 6 OF 9 HCA COPYRIGHT 2003 ACS on STN
 131:123053 1,2,3-Triazole compounds, their preparation, and organic
 electroluminescent device using them. Enomoto, Kazuhiro (Sharp Corp.,
 Japan). Jpn. Kokai Tokkyo Koho JP 11199567 A2 19990727 Heisei,
 17 pp. (Japanese). CODEN: JKXXAF. APPLICATION: JP 1998-6126 19980114.

GI



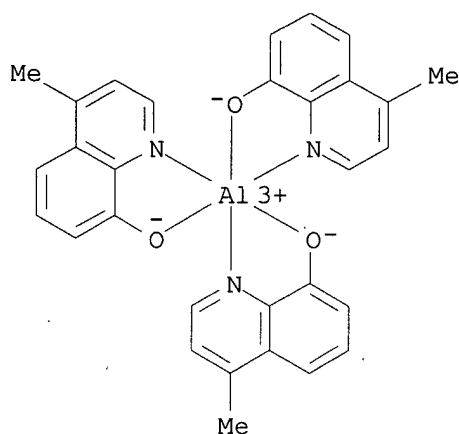
AB The compds. I [Ar, Ar1 = C6-12 (un)substituted arylene; R1, R2 = H, C1-4
 alkyl, (un)substituted aryl; X = O, S, (CH2)n, NR3, CHR4; R3 = H, C1-8
 alkyl, (un)substituted Ph, methallyl, allyl; R4 = H, C1-8 alkyl,
 (un)substituted phenyl; n = 0-2] are prep'd. by treatment of R1COCOR2 (R1,
 R2 = same as above) with H2NNHArXAr1NHNH2 (Ar, Ar1, X = same as above) or
 N(C6H4NHNH2-4)3 preferably in the presence of quaternary ammonium salts..
 An org. electroluminescent device comprising a cathode, hole injection
 transport layer contg. I, a luminescent layer, and an anode is also
 claimed. The electroluminescent device can be operated at a low voltage
 and is stable to H2O, O2, light, heat, etc.

IT 136779-65-2

RL: DEV (Device component use); USES (Uses)
 (prepn. of triazole compds. as hole-transporting agents for
 electroluminescent devices)

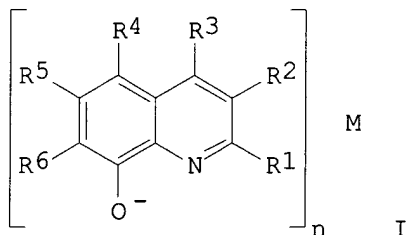
RN 136779-65-2 HCA

CN Aluminum, tris(4-methyl-8-quinolinolato-.kappa.N1,.kappa.O8)-, (OC-6-21)-
 (9CI) (CA INDEX NAME)



L31 ANSWER 7 OF 9 HCA COPYRIGHT 2003 ACS on STN
 121:220266 quinolinol metal compound used in electroluminescence device.
 Uchida, Manabu; Izumisawa, Jusho; Uchino, Masazumi; Furukawa, Kenji
 (Chisso Corp, Japan). Jpn. Kokai Tokkyo Koho JP 06145146 A2
19940524 Heisei, 10 pp. (Japanese). CODEN: JKXXAF. APPLICATION:
 JP 1992-322817 19921106.

GI



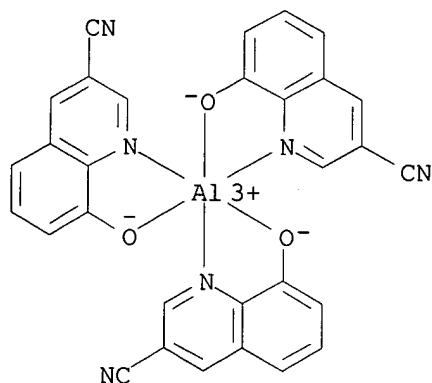
AB The title compd has formula I (R1-6 = H, F, cyano; at least 1 of R1-6 is F or cyano; M = metal; n = 1-4). By changing substituent, its position and no. or metal, compds. with different color can be obtained.

IT **158241-85-1P**, Aluminum tris(3-cyano-8-quinolinolate)

RL: SPN (Synthetic preparation); PREP (Preparation)
 (prepn. of)

RN 158241-85-1 HCA

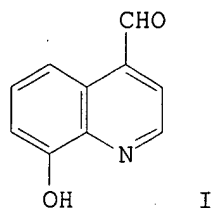
CN Aluminum, tris(8-hydroxy-3-quinolinecarbonitrilato-N1,O8)- (9CI) (CA
 INDEX NAME)



L31 ANSWER 8 OF 9 HCA COPYRIGHT 2003 ACS on STN

115:256438 Metal complexes of the alkaloid 4-formyl-8-hydroxyquinoline occurring in the timber of *Broussonetia zeylanica* (Thw.) corner. Ileperuma, O. A.; Senarathna, R. C.; Meedeniya, M. M. C. (Dep. Chem., Univ. Peradeniya, Peradeniya, Sri Lanka). *Journal of the National Science Council of Sri Lanka*, 17(2), 111-15 (English) 1989. CODEN: JNSCBH. ISSN: 0300-9254.

GI



AB Several complexes of the ligand 4-formyl-8-hydroxyquinoline (I) with the metal ions, Ni^{2+} , Zn^{2+} , Cu^{2+} , Cd^{2+} , Mn^{2+} , Mg^{2+} , Al^{3+} , Fe^{3+} and MoO_2^{2+} have been synthesized. Their compn. have been characterized from elemental analyses and spectroscopic data. These studies may bear some relevance to the role of naturally occurring ligand in the metal ion translocation in plants.

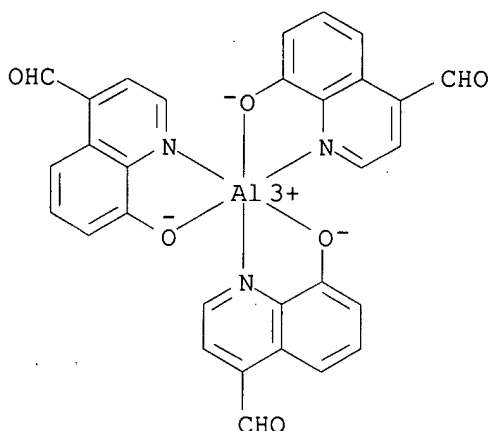
IT 137376-89-7P

RL: PREP (Preparation)

(prepn. of, occurrence in timber of *Broussonetia zeylanica* in relation to)

RN 137376-89-7 HCA

CN Aluminum, tris(8-hydroxy-4-quinolinecarboxaldehydato-N1,O8)- (9CI) (CA INDEX NAME)



L31 ANSWER 9 QF 9 HCA COPYRIGHT 2003 ACS on STN

115:196728 Model systems for gallium extraction. I. Structure and molecular dynamics of aluminum and gallium tris(oxinates). Schmidbaur, Hubert; Lettenbauer, Josef; Wilkinson, Dallas L.; Mueller, Gerhard; Kumberger, Otto (Anorg.-Chem. Inst., Tech. Univ. Munich, Garching, D-8046, Germany). Zeitschrift fuer Naturforschung, B: Chemical Sciences, 46(7), 901-11 (German) 1991. CODEN: ZNBSEN. ISSN: 0932-0776.

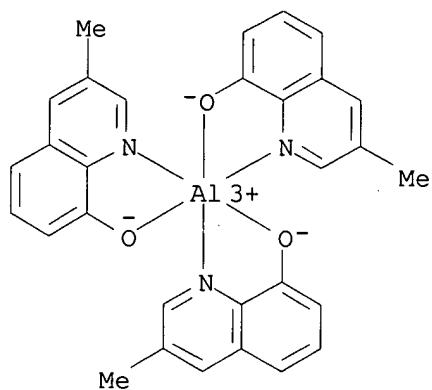
AB M(Ox)₃.L (OxH = 8-hydroxyquinoline and its 6 C-methylated derivs.; L = H₂O, MeOH; M = Al, Ga) were prepd. from aq. solns. of the metal chlorides or nitrates and an NH₄OAc buffer. Single crystal x-ray diffraction studies reveal a meridional tris(chelate) structure for (isomorphous) Al(Ox)₃.MeOH and Ga(Ox)₃.MeOH with distinct differences in the individual dimensions. (The MeOH mols. form strong H bonds with 1 of the O atoms.). For these species and those of the substituted ligands 3-MeOx, 4-MeOx, 5-MeOx, 6-MeOx, and 7-MeOx a similar meridional structure was confirmed by low temp. 1H NMR spectroscopy, which showed 3 inequivalent sets of ligands in each case. The collapse of these signals at elevated temps. indicates a ligand-equilibrating process, with the mechanism probably comprising a dissocn. of a pyridine function from the metal, to give a fluxional 5-coordinate species with free rotation about the intact M-O bond, and an M-N recombination at a random octahedral site. For the 2-MeOx ligands, the facial structure is preferred at lower temp., but with the meridional isomer present as a component of an equil. This indicates the strong steric influence of substituents in 2-position of the 8-oxyquinoline.

IT 136711-26-7P 136779-65-2P

RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation) (prepn. and NMR of)

RN 136711-26-7 HCA

CN Aluminum, tris(3-methyl-8-quinolinolato-.kappa.N1,.kappa.O8)-, (OC-6-21)-(9CI) (CA INDEX NAME)



RN 136779-65-2 HCA

CN Aluminum, tris(4-methyl-8-quinolinolato-.kappa.N1,.kappa.O8)-, (OC-6-21)-
(9CI) (CA INDEX NAME)

